

10540421

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LOGINID:ssspta1612bxr

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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

| | | | | |
|------|----|-----|----|---|
| NEWS | 1 | | | Web Page for STN Seminar Schedule - N. America |
| NEWS | 2 | OCT | 02 | CA/CAPLUS enhanced with pre-1907 records from Chemisches Zentralblatt |
| NEWS | 3 | OCT | 19 | BEILSTEIN updated with new compounds |
| NEWS | 4 | NOV | 15 | Derwent Indian patent publication number format enhanced |
| NEWS | 5 | NOV | 19 | WPIX enhanced with XML display format |
| NEWS | 6 | NOV | 30 | ICSD reloaded with enhancements |
| NEWS | 7 | DEC | 04 | LINPADOCDB now available on STN |
| NEWS | 8 | DEC | 14 | BEILSTEIN pricing structure to change |
| NEWS | 9 | DEC | 17 | USPATOLD added to additional database clusters |
| NEWS | 10 | DEC | 17 | IMSDRUGCONF removed from database clusters and STN |
| NEWS | 11 | DEC | 17 | DGENE now includes more than 10 million sequences |
| NEWS | 12 | DEC | 17 | TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment |
| NEWS | 13 | DEC | 17 | MEDLINE and LMEALINE updated with 2008 MeSH vocabulary |
| NEWS | 14 | DEC | 17 | CA/CAPLUS enhanced with new custom IPC display formats |
| NEWS | 15 | DEC | 17 | STN Viewer enhanced with full-text patent content from USPATOLD |
| NEWS | 16 | JAN | 02 | STN pricing information for 2008 now available |
| NEWS | 17 | JAN | 16 | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS | 18 | JAN | 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS | 19 | JAN | 28 | MARPAT searching enhanced |
| NEWS | 20 | JAN | 28 | USGENE now provides USPTO sequence data within 3 days of publication |
| NEWS | 21 | JAN | 28 | TOXCENTER enhanced with reloaded MEDLINE segment |
| NEWS | 22 | JAN | 28 | MEDLINE and LMEALINE reloaded with enhancements |
| NEWS | 23 | FEB | 08 | STN Express, Version 8.3, now available |
| NEWS | 24 | FEB | 20 | PCI now available as a replacement to DPCI |
| NEWS | 25 | FEB | 25 | IFIREF reloaded with enhancements |
| NEWS | 26 | FEB | 25 | IMSPRODUCT reloaded with enhancements |
| NEWS | 27 | FEB | 29 | WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification |

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability

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NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008

| | | |
|----------------------|------------|---------|
| => file reg | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
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STRUCTURE FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\asdgc.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Updated Search

10540421

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 22:14:41 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 303 TO ITERATE

100.0% PROCESSED 303 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5016 TO 7104

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 22:14:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6538 TO ITERATE

100.0% PROCESSED 6538 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

180.20

180.41

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

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FILE COVERS 1907 - 11 Mar 2008 VOL 148 ISS 11

FILE LAST UPDATED: 10 Mar 2008 (20080310/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Updated Search

10540421

=> s 13

L4 2 L3

=> s 14 and shinya, y?/au

58 SHINYA, Y?/AU

L5 0 L4 AND SHINYA, Y?/AU

=> s 14 and watanabe, t?/au

22474 WATANABE, T?/AU

L6 2 L4 AND WATANABE, T?/AU

=> d 16, ibib abs hitstr, 1-2

L6 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:872791 HCAPLUS

DOCUMENT NUMBER: 141:350046

TITLE: Preparation of novel crystal of fluorobenzamide derivative

INVENTOR(S): Yoshida, Shinya; Watanabe, Toshihiro; Marumo, Kiyotaka; Yamaguchi, Sou

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

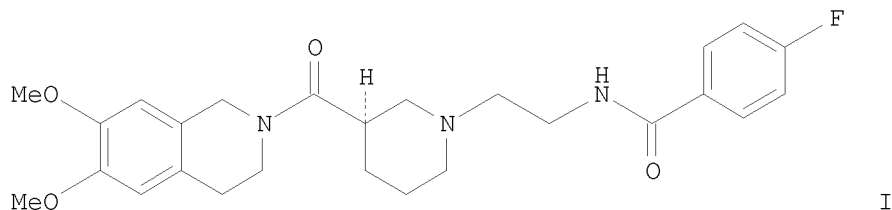
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---------------------|----------|------------------|------------|
| ----- | ---- | ----- | ----- | ----- |
| WO 2004089933 | A1 | 20041021 | WO 2004-JP4794 | 20040401 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2519882 | A1 | 20041021 | CA 2004-2519882 | 20040401 |
| EP 1609788 | A1 | 20051228 | EP 2004-725182 | 20040401 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR | | | | |
| CN 1771245 | A | 20060510 | CN 2004-80009451 | 20040401 |
| IN 2005DN04378 | A | 20070105 | IN 2005-DN4378 | 20050927 |
| MX 2005PA10603 | A | 20060725 | MX 2005-PA10603 | 20050930 |
| US 2007129357 | A1 | 20070607 | US 2005-552019 | 20051003 |
| PRIORITY APPLN. INFO.: | | | JP 2003-99411 | A 20030402 |
| | | | WO 2004-JP4794 | W 20040401 |
| OTHER SOURCE(S): | CASREACT 141:350046 | | | |
| GI | | | | |

Updated Search

10540421



AB A novel crystal of (R)-(-)-N-[2-[3-[(6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidino]ethyl]-4-fluorobenzamide (I) monophosphate, which is known as a preventive and/or remedy for ischemic diseases such as angina pectoris and myocardial infarction and cardiovascular diseases such as ischemic heart failure and arrhythmia, was prepared and characterized by X-ray diffraction spectra and DSC. Two crystal forms (α and β crystal forms) of compound I were prepared. α Crystal form of compound I exhibited excellent moisture adsorption property and is advantageous for handling and formulation. Thus, 206.4 g (R)-1-[2-[(4-fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid was treated with 810 mL DMF and 120.8 g 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline monohydrochloride, stirred, cooled, treated with 53.22 g Et₃N at $\leq 12^\circ$, treated with 217 mL DMF and then successively with 21.32 g 1H-1,2,3-benzotriazole and 121.0 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride at $\leq 5^\circ$, and stirred at $0-4^\circ$ for 15.5 h, and treated with 340 mL H₂O, 2,000 mL EtOAc, and 550 mL 8% (W/V) aqueous NaOH solution to give, after workup and concentration, crude free base I (83.9% purity). I (11.90 g) was dissolved in ethanol to a total weight of 97.8 g, treated with 5 mL ethanol, 0.47 g H₂O, and 0.86 g 85% H₃PO₄, and then with 5 mL ethanol, stirred at 30° overnight, and filtered to give, after washing the crystals with ethanol and drying, 3.38 g I monophosphate (α crystal form).

IT 721452-52-4P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid ethyl ester 721452-55-7P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel crystal of fluorobenzamide monophosphate derivative having

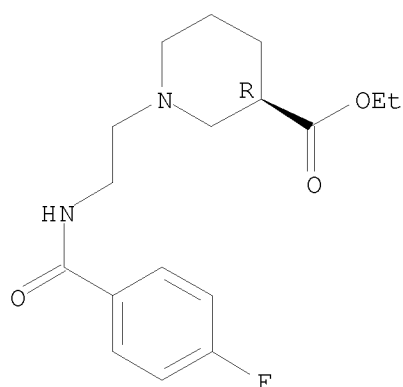
excellent moisture adsorption property)

RN 721452-52-4 HCAPLUS

CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

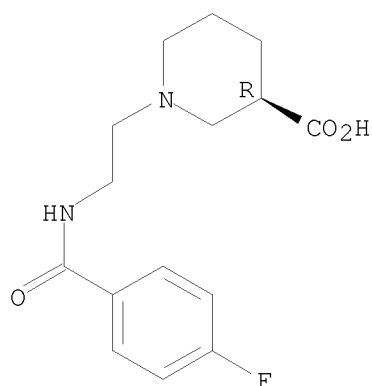
10540421



RN 721452-55-7 HCAPLUS

CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)-
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:565208 HCAPLUS

DOCUMENT NUMBER: 141:106387

TITLE: Isoquinoline derivatives containing benzamide moiety
and process for their preparation

INVENTOR(S): Yoshida, Shinya; Watanabe, Toshihiro;

Marumo, Kiyotaka; Kakefuda, Akio

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

Updated Search

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|-------------------|--|------------|
| ----- | ---- | ----- | ----- | ----- |
| WO 2004058710 | A1 | 20040715 | WO 2003-JP16582 | 20031224 |
| W: | | | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | |
| RW: | | | BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | |
| CA 2511989 | A1 | 20040715 | CA 2003-2511989 | 20031224 |
| AU 2003292757 | A1 | 20040722 | AU 2003-292757 | 20031224 |
| CN 1753870 | A | 20060329 | CN 2003-80109919 | 20031224 |
| IN 2005DN02787 | A | 20070105 | IN 2005-DN2787 | 20050623 |
| US 2006084807 | A1 | 20060420 | US 2005-540421 | 20050624 |
| KR 758522 | B1 | 20070914 | KR 2005-711965 | 20050624 |
| PRIORITY APPLN. INFO.: | | | JP 2002-375153 | A 20021225 |
| | | | WO 2003-JP16582 | W 20031224 |
| OTHER SOURCE(S): | | MARPAT 141:106387 | | |
| GI | | | | |

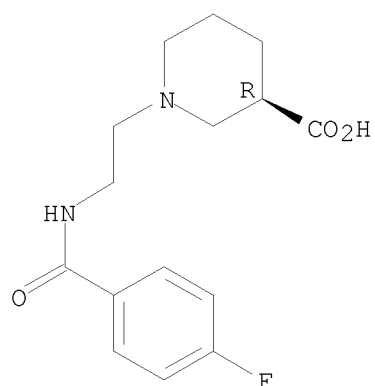
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Process for the preparation of compds. I [R3 =, R4 = H, alkyl, alkoxy; Ar = (un)substituted aryl] and compds. II [R1 = H, alkyl, benzyl; R2 = H, protecting group of amino; Ar = (un)substituted aryl] were provided. For example, a mixture of compound (R)-II [R1 = Ethyl; R2 = H; Ar = 4-fluorophenyl] (37.94 g), e.g., prepared from (R)-piperidine-3-carboxylic acid Et ester L-tartaric acid salt in 4 steps, and 1 M aqueous NaOH (177 mL) in EtOH (100 mL) stirred at room temperature for 1 h. After treating the reaction with HCl to acidic pH, the solvent was azeotropically removed by toluene. Then, to a solution of the resulting residue in DMF (250 mL) were added 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride (21.66 g), HOBT (7.97 g) and WSC hydrochloride (27.14 g) at 10 °C. The reaction was stirred at room temperature for 3 h, aqueous work-up followed by treatment with 85% phosphoric acid (13.65 g) in EtOH (500 mL) afforded claimed compound III phosphoric acid salt (44.25 g). Of note, compds. I are useful for prophylaxis and/or treatment of myocardial infarction, congestive heart failure, etc. (no data). The disclosed process employs less hazardous solvent.

IT 721452-55-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (N-benzoylaminoethylation of nipecotic acid derivs. using dihydrooxazoles)
 RN 721452-55-7 HCAPLUS
 CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)- (CA INDEX NAME)

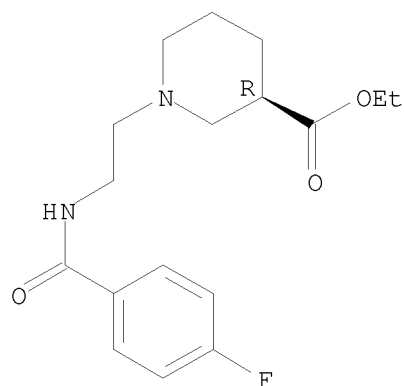
Absolute stereochemistry.

10540421



IT 721452-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of isoquinoline derivs. via N-fluorobenzoylation of
tetrahydroisoquinoline derivs.)
RN 721452-52-4 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl
ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



=> file caold
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 13.59 | 194.00 |

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| -1.60 | -1.60 |

CA SUBSCRIBER PRICE

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

L4 2 S L3
L5 0 S L4 AND SHINYA, Y?/AU
L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

=> s l3

L7 0 L3

=> file reg

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.46 | 194.46 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -1.60 |

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
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Updated Search

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STRUCTURE FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\421.str

L8 STRUCTURE UPLOADED

=> d l8

L8 HAS NO ANSWERS

L8 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l8

SAMPLE SEARCH INITIATED 22:16:48 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 309 TO ITERATE

100.0% PROCESSED 309 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5126 TO 7234

PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=> s l8 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 22:16:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6564 TO ITERATE

100.0% PROCESSED 6564 ITERATIONS 9 ANSWERS

SEARCH TIME: 00.00.01

L10 9 SEA SSS FUL L8

Updated Search

10540421

=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

L4 2 S L3

L5 0 S L4 AND SHINYA, Y?/AU

L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

L7 0 S L3

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008

L8 STRUCTURE UPLOADED

L9 0 S L8

L10 9 S L8 FULL

=> s l10 not l6

NUMERIC VALUE NOT VALID 'WATANABE, T?'

0 WATANABE, T?/AU

L11 9 L10 NOT L6

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

184.43

378.89

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-1.60

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008

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FILE COVERS 1907 - 11 Mar 2008 VOL 148 ISS 11

FILE LAST UPDATED: 10 Mar 2008 (20080310/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

Updated Search

10540421

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l11

L12 6 L11

=> s l12 and yoshida, s?/au

9851 YOSHIDA, S?/AU

L13 2 L12 AND YOSHIDA, S?/AU

=> d l13, ibib abs hitstr, 1-6

L13 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:872791 HCAPLUS

DOCUMENT NUMBER: 141:350046

TITLE: Preparation of novel crystal of fluorobenzamide derivative

INVENTOR(S): Yoshida, Shinya; Watanabe, Toshihiro; Marumo, Kiyotaka; Yamaguchi, Sou

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

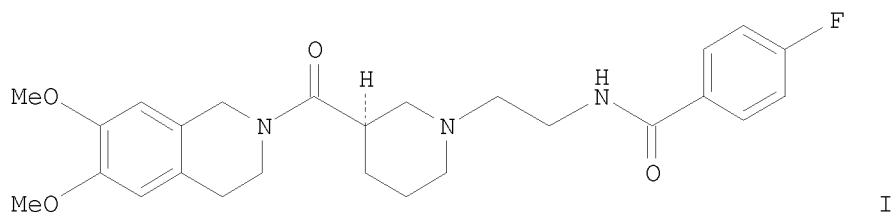
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|---------------------|------------------|------------|
| WO 2004089933 | A1 | 20041021 | WO 2004-JP4794 | 20040401 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2519882 | A1 | 20041021 | CA 2004-2519882 | 20040401 |
| EP 1609788 | A1 | 20051228 | EP 2004-725182 | 20040401 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR | | | | |
| CN 1771245 | A | 20060510 | CN 2004-80009451 | 20040401 |
| IN 2005DN04378 | A | 20070105 | IN 2005-DN4378 | 20050927 |
| MX 2005PA10603 | A | 20060725 | MX 2005-PA10603 | 20050930 |
| US 2007129357 | A1 | 20070607 | US 2005-552019 | 20051003 |
| PRIORITY APPLN. INFO.: | | | JP 2003-99411 | A 20030402 |
| | | | WO 2004-JP4794 | W 20040401 |
| OTHER SOURCE(S): | | CASREACT 141:350046 | | |
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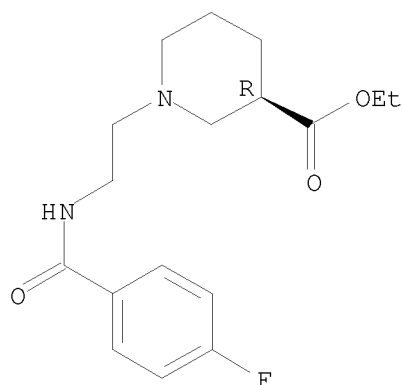
Updated Search



- AB A novel crystal of (R)-(-)-N-[2-[3-[(6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidino]ethyl]-4-fluorobenzamide (I) monophosphate, which is known as a preventive and/or remedy for ischemic diseases such as angina pectoris and myocardial infarction and cardiovascular diseases such as ischemic heart failure and arrhythmia, was prepared and characterized by X-ray diffraction spectra and DSC. Two crystal forms (α and β crystal forms) of compound I were prepared
- α Crystal form of compound I exhibited excellent moisture adsorption property and is advantageous for handling and formulation. Thus, 206.4 g (R)-1-[2-[(4-fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid was treated with 810 mL DMF and 120.8 g 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline monohydrochloride, stirred, cooled, treated with 53.22 g Et₃N at $\leq 12^\circ$, treated with 217 mL DMF and then successively with 21.32 g 1H-1,2,3-benzotriazole and 121.0 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride at $\leq 5^\circ$, and stirred at $0-4^\circ$ for 15.5 h, and treated with 340 mL H₂O, 2,000 mL EtOAc, and 550 mL 8% (W/V) aqueous NaOH solution to give, after workup and concentration, crude free base I (83.9% purity). I (11.90 g) was dissolved in ethanol to a total weight of 97.8 g, treated with 5 mL ethanol, 0.47 g H₂O, and 0.86 g 85% H₃PO₄, and then with 5 mL ethanol, stirred at 30° overnight, and filtered to give, after washing the crystals with ethanol and drying, 3.38 g I monophosphate (α crystal form).
- IT 721452-52-4P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid ethyl ester 721452-55-7P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid
- RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
- (preparation of novel crystal of fluorobenzamide monophosphate derivative having excellent moisture adsorption property)
- RN 721452-52-4 HCAPLUS
- CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.

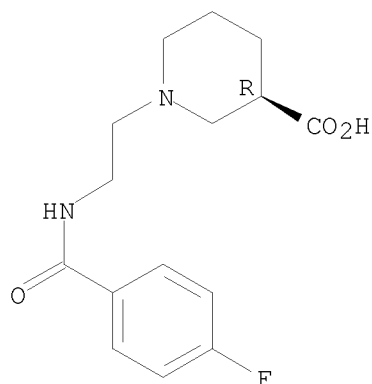
10540421



RN 721452-55-7 HCAPLUS

CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)-
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:565208 HCAPLUS

DOCUMENT NUMBER: 141:106387

TITLE: Isoquinoline derivatives containing benzamide moiety
and process for their preparation

INVENTOR(S): Yoshida, Shinya; Watanabe, Toshihiro;
Marumo, Kiyotaka; Kakefuda, Akio

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

Updated Search

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|-------------------|--|------------|
| ----- | ---- | ----- | ----- | ----- |
| WO 2004058710 | A1 | 20040715 | WO 2003-JP16582 | 20031224 |
| W: | | | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | |
| RW: | | | BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | |
| CA 2511989 | A1 | 20040715 | CA 2003-2511989 | 20031224 |
| AU 2003292757 | A1 | 20040722 | AU 2003-292757 | 20031224 |
| CN 1753870 | A | 20060329 | CN 2003-80109919 | 20031224 |
| IN 2005DN02787 | A | 20070105 | IN 2005-DN2787 | 20050623 |
| US 2006084807 | A1 | 20060420 | US 2005-540421 | 20050624 |
| KR 758522 | B1 | 20070914 | KR 2005-711965 | 20050624 |
| PRIORITY APPLN. INFO.: | | | JP 2002-375153 | A 20021225 |
| | | | WO 2003-JP16582 | W 20031224 |
| OTHER SOURCE(S): | | MARPAT 141:106387 | | |
| GI | | | | |

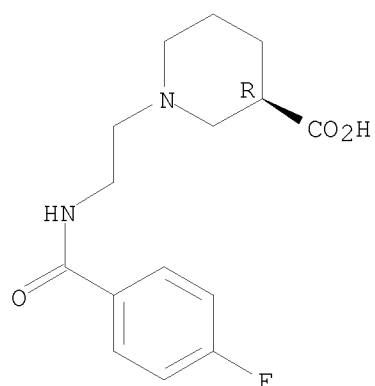
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Process for the preparation of compds. I [R3 =, R4 = H, alkyl, alkoxy; Ar = (un)substituted aryl] and compds. II [R1 = H, alkyl, benzyl; R2 = H, protecting group of amino; Ar = (un)substituted aryl] were provided. For example, a mixture of compound (R)-II [R1 = Ethyl; R2 = H; Ar = 4-fluorophenyl] (37.94 g), e.g., prepared from (R)-piperidine-3-carboxylic acid Et ester L-tartaric acid salt in 4 steps, and 1 M aqueous NaOH (177 mL) in EtOH (100 mL) stirred at room temperature for 1 h. After treating the reaction with HCl to acidic pH, the solvent was azeotropically removed by toluene. Then, to a solution of the resulting residue in DMF (250 mL) were added 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride (21.66 g), HOBT (7.97 g) and WSC hydrochloride (27.14 g) at 10 °C. The reaction was stirred at room temperature for 3 h, aqueous work-up followed by treatment with 85% phosphoric acid (13.65 g) in EtOH (500 mL) afforded claimed compound III phosphoric acid salt (44.25 g). Of note, compds. I are useful for prophylaxis and/or treatment of myocardial infarction, congestive heart failure, etc. (no data). The disclosed process employs less hazardous solvent.

IT 721452-55-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (N-benzoylaminoethylation of nipecotic acid derivs. using dihydrooxazoles)
 RN 721452-55-7 HCAPLUS
 CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)- (CA INDEX NAME)

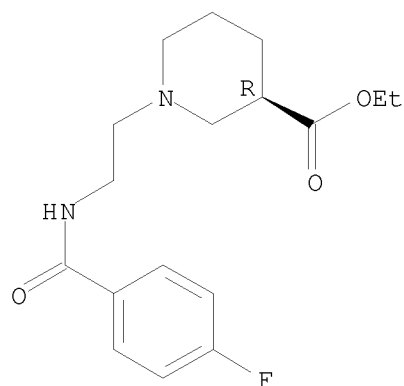
Absolute stereochemistry.

10540421



IT 721452-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of isoquinoline derivs. via N-fluorobenzoylation of
tetrahydroisoquinoline derivs.)
RN 721452-52-4 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl
ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

Updated Search

10540421

L4 2 S L3
L5 0 S L4 AND SHINYA, Y?/AU
L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008
L7 0 S L3

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
L8 STRUCTURE UPLOADED
L9 0 S L8
L10 9 S L8 FULL
L11 9 S L10 NOT L6

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008
L12 6 S L11
L13 2 S L12 AND YOSHIDA, S?/AU

=> s l12 not l13
L14 4 L12 NOT L13

=> s l14 and watanabe, t?/au
22474 WATANABE, T?/AU
L15 0 L14 AND WATANABE, T?/AU

=> s l14 and marumo, k?/au
217 MARUMO, K?/AU
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=> s l14 and kakefuda, a?/au
45 KAKEFUDA, A?/AU
L17 0 L14 AND KAKEFUDA, A?/AU

=> s l11/uses
6 L11
6920858 USES/RL
L18 2 L11/USES
(L11 (L) USES/RL)

=> d l18, ibib abs hitstr, 1-2

L18 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:405003 HCAPLUS
DOCUMENT NUMBER: 146:155278
TITLE: Non-stochastic and stochastic linear indices of the
molecular pseudograph's atom-adjacency matrix: a novel
approach for computational in silico screening and
"rational" selection of new lead antibacterial agents
AUTHOR(S): Marrero-Ponce, Yovani; Marrero, Ricardo Medina;
Torrens, Francisco; Martinez, Yamile; Bernal, Milagros
Garcia; Zaldivar, Vicente Romero; Castro, Eduardo A.;
Abalo, Ricardo Grau
CORPORATE SOURCE: Department of Pharmacy, Faculty of Chemical-Pharmacy,
Central University of Las Villas, Santa Clara, 54830,
Cuba
SOURCE: Journal of Molecular Modeling (2006), 12(3), 255-271
CODEN: JMMOFK; ISSN: 0948-5023

Updated Search

10540421

URL: <http://www.springerlink.com/media/ef6tmfk36j3ttmb97wlh/contributions/1/2/v/4/12v47qr26320v870.pdf>

PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

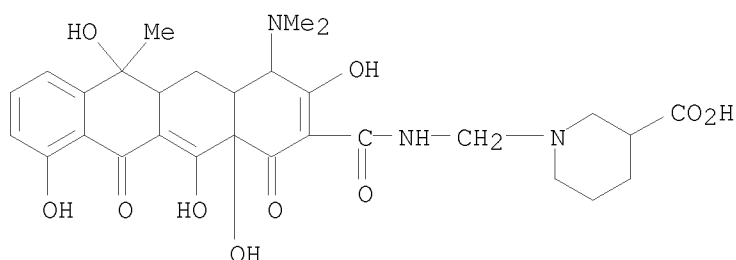
AB A novel approach (TOMOCOMD-CARDD) to computer-aided rational drug design is illustrated. This approach is based on the calcn. of the non-stochastic and stochastic linear indexes of the mol. pseudograph's atom-adjacency matrix representing mol. structures. These TOMOCOMD-CARDD descriptors are introduced for the computational (virtual) screening and rational selection of new lead antibacterial agents using linear discrimination anal. The two structure-based antibacterial-activity classification models, including non-stochastic and stochastic indexes, classify correctly 91.61% and 90.75%, resp., of 1525 chems. in training sets. These models show high Matthews correlation coeffs. (MCC = 0.84 and 0.82). An external validation process was carried out to assess the robustness and predictive power of the model obtained. These QSAR models permit the correct classification of 91.49% and 89.31% of 505 compds. in an external test set, yielding MCCs of 0.84 and 0.79, resp. The TOMOCOMD-CARDD approach compares satisfactorily with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, an in silico screening of 87 new chems. reported in the antiinfective field with antibacterial activities is developed showing the ability of the TOMOCOMD-CARDD models to identify new lead antibacterial compds.

IT 15301-82-3, Pecocycline

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel QSAR model TOMOCOMD-CARDD in computer-aided rational drug design for selection of new lead antibacterial agents using linear discrimination anal.)

RN 15301-82-3 HCAPLUS

CN 3-Piperidinecarboxylic acid, (4S,4aS,5aS,6S,12aS)-1-[[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenyl]carbonyl]amino]methyl]- (CA INDEX NAME)



REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:244333 HCAPLUS

DOCUMENT NUMBER: 143:307

TITLE: Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising

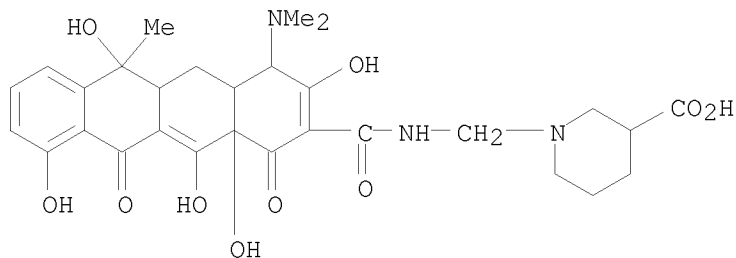
Updated Search

10540421

AUTHOR(S): approach for modeling of antibacterial activity
Marrero-Ponce, Yovani; Medina-Marrero, Ricardo;
Torrens, Francisco; Martinez, Yamile; Romero-Zaldivar,
Vicente; Castro, Eduardo A.
CORPORATE SOURCE: Department of Pharmacy, Faculty of Chemical-Pharmacy,
Central University of Las Villas, Santa Clara, 54830,
Cuba
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(8),
2881-2899
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The Topol. Mol. Computer Design (TOMOCOMD-CARDD) approach has been introduced for the classification and design of antimicrobial agents using computer-aided mol. design. For this propose, atom, atom-type, and total quadratic indexes have been generalized to codify chemical structure information. In this sense, stochastic quadratic indexes have been introduced for the description of the mol. structure. These stochastic fingerprints are based on a simple model for the intramol. movement of all valence-bond electrons. In this work, a complete data set containing 1006 antimicrobial agents is collected and presented. Two structure-based antibacterial activity classification models have been generated. The models (including nonstochastic and stochastic indexes) classify correctly more than 90% of 1525 compds. in training sets. These models permit the correct classification of 92.28% and 89.31% of 505 compds. in an external test sets. The approach, also, satisfactorily compares with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, a virtual screening of 87 new compds. reported in the anti-infective field with antibacterial activities is developed showing the ability of the models to identify new leads as antibacterial.

IT 15301-82-3, Pecocycline
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints as promising approach for modeling antibacterial activity)
RN 15301-82-3 HCAPLUS
CN 3-Piperidinecarboxylic acid, (4S,4aS,5aS,6S,12aS)-1-[[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenyl]carbonyl]amino]methyl]- (CA INDEX NAME)



REFERENCE COUNT: 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

10540421

=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

L4 2 S L3

L5 0 S L4 AND SHINYA, Y?/AU

L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

L7 0 S L3

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008

L8 STRUCTURE UPLOADED

L9 0 S L8

L10 9 S L8 FULL

L11 9 S L10 NOT L6

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008

L12 6 S L11

L13 2 S L12 AND YOSHIDA, S?/AU

L14 4 S L12 NOT L13

L15 0 S L14 AND WATANABE, T?/AU

L16 0 S L14 AND MARUMO, K?/AU

L17 0 S L14 AND KAKEFUDA, A?/AU

L18 2 S L11/USES

=> file caold

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| | ENTRY | SESSION |
| FULL ESTIMATED COST | 29.87 | 408.76 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
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| CA SUBSCRIBER PRICE | -3.20 | -4.80 |

FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

Updated Search

10540421

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l11

L19 1 L11

=> d l19, all, 1

L19 ANSWER 1 OF 1 CAOLD COPYRIGHT 2008 ACS on STN

AN CA63:13180h CAOLD

TI pyrenylmethyamines

AU Clarke, Robert LaGrone; Buck, J. S.

PA Sterling Drug Inc.

DT Patent

| | PATENT NO. | KIND | DATE |
|--|------------|------|------|
|--|------------|------|------|

| | ----- | ----- | ---- |
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| | | | |
|----|------------|--|------|
| PI | US 3198835 | | 1965 |
|----|------------|--|------|

| | | | | | | |
|----|-------------|-------------|-----------|-----------|-------------|-----------|
| IT | 897-41-6 | 1729-05-1 | 3590-94-1 | 3590-95-2 | 3590-96-3 | |
| | 3590-97-4 | 3590-98-5 | 3590-99-6 | 3591-00-2 | 3591-01-3 | 3591-02-4 |
| | 3591-03-5 | 3712-78-5 | 3712-79-6 | 3765-68-2 | 3786-54-7 | 3786-55-8 |
| | 3786-56-9 | 3786-57-0 | 3786-59-2 | 3786-60-5 | 3786-61-6 | 3786-62-7 |
| | 3786-63-8 | 3786-66-1 | 3786-67-2 | 3804-54-4 | 3804-55-5 | 3806-02-8 |
| | 3840-95-7 | 3874-63-3 | 4914-39-0 | 6614-22-8 | 101201-45-0 | |
| | 104298-70-6 | 106439-18-3 | | | | |

=> FIL REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
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| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -4.80 |

FILE 'REGISTRY' ENTERED AT 22:19:57 ON 11 MAR 2008

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STRUCTURE FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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Updated Search

10540421

conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> S 6614-22-8/RN

L20 1 6614-22-8/RN

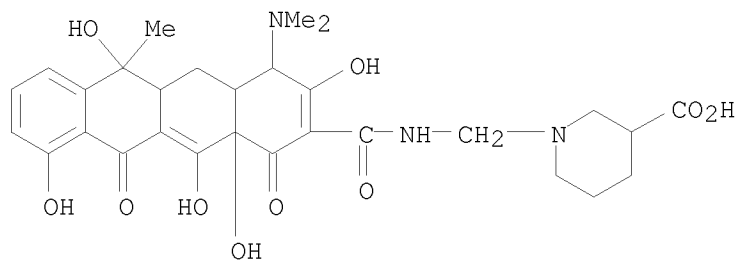
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SET COMMAND COMPLETED

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THE ESTIMATED COST FOR THIS REQUEST IS 6.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 6614-22-8 REGISTRY
CN Nipecotic acid, 1-[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamido]methyl]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)
MF C29 H35 N3 O10 . Cl H
LC STN Files: CA, CAOLD, CAPLUS, USPATOLD
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)
CRN (741608-18-4)



● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

Updated Search

10540421

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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=> file reg

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 2.46 | 412.83 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -4.80 |

FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
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DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\2ef.str

L21 STRUCTURE UPLOADED

=> d 121

L21 HAS NO ANSWERS
L21 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 121

Updated Search

10540421

SAMPLE SEARCH INITIATED 22:21:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 8538 TO ITERATE

23.4% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 165221 TO 176299
PROJECTED ANSWERS: 0 TO 0

L22 0 SEA SSS SAM L21

=> s l21 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 22:21:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 170590 TO ITERATE

100.0% PROCESSED 170590 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.03

L23 3 SEA SSS FUL L21

=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

L4 2 S L3
L5 0 S L4 AND SHINYA, Y?/AU
L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

L7 0 S L3

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008

L8 STRUCTURE UPLOADED
L9 0 S L8
L10 9 S L8 FULL
L11 9 S L10 NOT L6

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008

L12 6 S L11
L13 2 S L12 AND YOSHIDA, S?/AU
L14 4 S L12 NOT L13
L15 0 S L14 AND WATANABE, T?/AU
L16 0 S L14 AND MARUMO, K?/AU
L17 0 S L14 AND KAKEFUDA, A?/AU
L18 2 S L11/USES

Updated Search

10540421

FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008
L19 1 S L11

FILE 'REGISTRY' ENTERED AT 22:19:57 ON 11 MAR 2008
L20 1 S 6614-22-8/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
L21 STRUCTURE UPLOADED
L22 0 S L21
L23 3 S L21 FULL

=> s l23 not l3
L24 1 L23 NOT L3

=> s l24 not l11
L25 1 L24 NOT L11

=> s l24 not l18
'USES' IS NOT A VALID CROSSOVER QUALIFIER FOR L11
Answer sets created in a different file may be field qualified with a
limited set of qualifiers. Enter HELP CROSSOVER at an arrow prompt
(=>) for specific information.

=> file hcaplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|---------------------|------------------|
| FULL ESTIMATED COST | 179.28 | 592.11 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|---------------------|------------------|
| CA SUBSCRIBER PRICE | 0.00 | -4.80 |

FILE 'HCAPLUS' ENTERED AT 22:22:31 ON 11 MAR 2008
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FILE COVERS 1907 - 11 Mar 2008 VOL 148 ISS 11
FILE LAST UPDATED: 10 Mar 2008 (20080310/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

Updated Search

10540421

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 125

L26 2 L25

=> s 126 and yoshida, s?/au

9851 YOSHIDA, S?/AU

L27 0 L26 AND YOSHIDA, S?/AU

=> s 126 and watanabe, t?/au

22474 WATANABE, T?/AU

L28 0 L26 AND WATANABE, T?/AU

=> s 126 and marumo, k?/au

217 MARUMO, K?/AU

L29 0 L26 AND MARUMO, K?/AU

=> s 126 and kakefuda, a?/au

45 KAKEFUDA, A?/AU

L30 0 L26 AND KAKEFUDA, A?/AU

=> d 126, ibib abs hitstr, 1-2

L26 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1228883 HCAPLUS

DOCUMENT NUMBER: 145:505447

TITLE: Preparation of high-conductance, calcium-sensitive potassium channel openers

INVENTOR(S): Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki; Hosaka, Toshihiro; Kono, Rikako

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 164pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

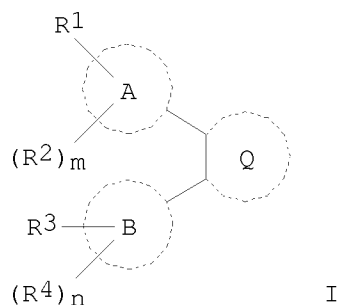
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|------------|
| ----- | ---- | ----- | ----- | ----- |
| JP 2006316054 | A | 20061124 | JP 2006-111427 | 20060414 |
| PRIORITY APPLN. INFO.: | | | JP 2005-117662 | A 20050415 |
| OTHER SOURCE(S): | MARPAT | 145:505447 | | |
| GI | | | | |

10540421



AB Title openers, useful for prophylactic and therapeutic treatment of urinary frequency, incontinence, asthma, and chronic obstructive pulmonary disease, are prepared from tricyclic compds. I [ring A = benzene, heterocycle; ring B = benzene, heterocycle, cycloalkane, cycloalkene; ring Q = halo- or (halo)alkyl-substituted pyrazole, isoxazole; R1, R3 = R5R6NCO, R5ONR6CO, R5R6NNHCO, R5CO, R5O, R5S, H, etc; R2, R4 = O, cyano, NO2, OH, alkoxy, halo, CO2H, etc.; R5, R6 = H, (un)substituted alkyl, (condensed) (un)substituted cycloalkyl, (un)substituted heterocyclyl, etc.; m, n = 0-2] are prepared Thus, deprotection of BOC-protected pyrazole derivative II (R = BOC) gave II (R = H), which inhibited K-induced bladder contraction with IC50 value of 1-3 μ M.

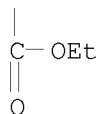
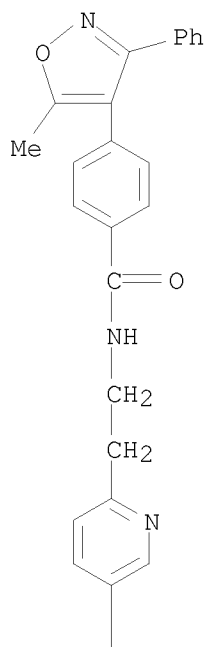
IT 850832-10-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazoles or isoxazoles as high-conductance, Ca²⁺-sensitive K⁺ channel openers for treatment of diseases)

RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)



L26 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:369275 HCAPLUS

DOCUMENT NUMBER: 142:430265

TITLE: Preparation of substituted pyrazoles and isoxazoles as large conductance Ca-activated K channel openers

INVENTOR(S): Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki; Hosaka, Toshihiro; Kono, Rikako

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: PCT Int. Appl., 224 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|----------|
| WO 2005037271 | A2 | 20050428 | WO 2004-JP15662 | 20041015 |
| WO 2005037271 | A3 | 20050901 | | |

10540421

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1675585 A2 20060705 EP 2004-792804 20041015

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

JP 2007518686 T 20070712 JP 2006-519291 20041015

US 2007060629 A1 20070315 US 2006-574529 20060404

PRIORITY APPLN. INFO.:

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JP 2004-17662 A 20040126

JP 2004-85143 A 20040323

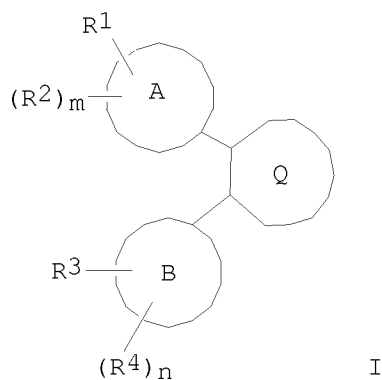
JP 2004-194172 A 20040630

US 2004-584451P P 20040701

WO 2004-JP15662 W 20041015

OTHER SOURCE(S): CASREACT 142:430265; MARPAT 142:430265

GI



AB Title compds. I [A = benzene, heterocycle; B = benzene, heterocycle, etc.; Q = pyrazolyl, isoxazolyl; R1, R3 = carboxamido, hydrazido, etc.; m, n = 0-2; R2, R4 = oxo, CN, NO2, etc.] are prepared For instance, 4,4,4-trifluoro-1-(4-methylphenyl)butane-1,3-dione is reacted with 3-methylphenylhydrazine•HCl (EtOH, reflux, 20 h) to give 1-(3-methylphenyl)-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazole (II). Data for over 400 compds. is given. The relaxation effect on K-induced contraction of isolated rabbit urinary bladder and the inhibitory effect on the rhythmic bladder contractions induced by substance P in anesthetized rats is provided for selected example compds. I are useful for the treatment of pollakiuria, urinary incontinence, etc.

IT 850832-10-9P

Updated Search

10540421

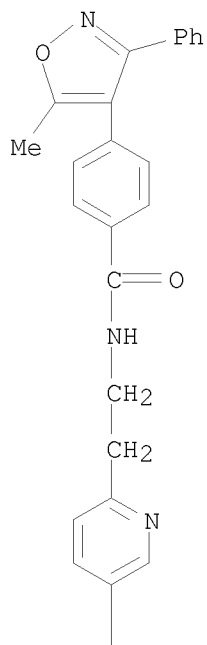
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of substituted pyrazoles and isoxazoles as large conductance
Ca-activated K channel openers)

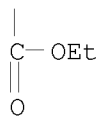
RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-
isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



=> file caold
COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

| SINCE FILE | TOTAL |
|------------|---------|
| ENTRY | SESSION |
| 13.59 | 605.70 |
| SINCE FILE | TOTAL |
| ENTRY | SESSION |
| -1.60 | -6.40 |

Updated Search

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FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

L4 2 S L3
L5 0 S L4 AND SHINYA, Y?/AU
L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

L7 0 S L3

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008

L8 STRUCTURE UPLOADED
L9 0 S L8
L10 9 S L8 FULL
L11 9 S L10 NOT L6

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008

L12 6 S L11
L13 2 S L12 AND YOSHIDA, S?/AU
L14 4 S L12 NOT L13
L15 0 S L14 AND WATANABE, T?/AU
L16 0 S L14 AND MARUMO, K?/AU
L17 0 S L14 AND KAKEFUDA, A?/AU
L18 2 S L11/USES

FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008

L19 1 S L11

Updated Search

10540421

FILE 'REGISTRY' ENTERED AT 22:19:57 ON 11 MAR 2008
L20 1 S 6614-22-8/RN
SET NOTICE 1 DISPLAY
SET NOTICE LOGIN DISPLAY

FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
L21 STRUCTURE UPLOADED
L22 0 S L21
L23 3 S L21 FULL
L24 1 S L23 NOT L3
L25 1 S L24 NOT L11

FILE 'HCAPLUS' ENTERED AT 22:22:31 ON 11 MAR 2008
L26 2 S L25
L27 0 S L26 AND YOSHIDA, S?/AU
L28 0 S L26 AND WATANABE, T?/AU
L29 0 S L26 AND MARUMO, K?/AU
L30 0 S L26 AND KAKEFUDA, A?/AU

FILE 'CAOLD' ENTERED AT 22:23:23 ON 11 MAR 2008

=> s 125
L31 0 L25

| | | |
|--|------------|---------|
| => file hcaplus | | |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.46 | 606.16 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | 0.00 | -6.40 |

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FILE LAST UPDATED: 10 Mar 2008 (20080310/ED)

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Updated Search

10540421

substance identification.

=> d his

(FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

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L5 0 S L4 AND SHINYA, Y?/AU

L6 2 S L4 AND WATANABE, T?/AU

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

L7 0 S L3

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008

L8 STRUCTURE UPLOADED

L9 0 S L8

L10 9 S L8 FULL

L11 9 S L10 NOT L6

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008

L12 6 S L11

L13 2 S L12 AND YOSHIDA, S?/AU

L14 4 S L12 NOT L13

L15 0 S L14 AND WATANABE, T?/AU

L16 0 S L14 AND MARUMO, K?/AU

L17 0 S L14 AND KAKEFUDA, A?/AU

L18 2 S L11/USES

FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008

L19 1 S L11

FILE 'REGISTRY' ENTERED AT 22:19:57 ON 11 MAR 2008

L20 1 S 6614-22-8/RN

SET NOTICE 1 DISPLAY

SET NOTICE LOGIN DISPLAY

FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008

L21 STRUCTURE UPLOADED

L22 0 S L21

L23 3 S L21 FULL

L24 1 S L23 NOT L3

L25 1 S L24 NOT L11

FILE 'HCAPLUS' ENTERED AT 22:22:31 ON 11 MAR 2008

L26 2 S L25

L27 0 S L26 AND YOSHIDA, S?/AU

L28 0 S L26 AND WATANABE, T?/AU

L29 0 S L26 AND MARUMO, K?/AU

L30 0 S L26 AND KAKEFUDA, A?/AU

Updated Search

10540421

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FILE 'HCAPLUS' ENTERED AT 22:23:39 ON 11 MAR 2008

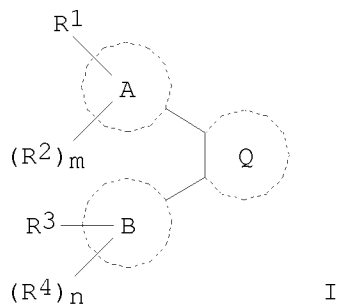
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(L25 (L) USES/RL)

=> d l32, ibib abs hitstr, 1-2

L32 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1228883 HCAPLUS
DOCUMENT NUMBER: 145:505447
TITLE: Preparation of high-conductance, calcium-sensitive
potassium channel openers
INVENTOR(S): Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki;
Hosaka, Toshihiro; Kono, Rikako
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 164pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|------------|
| JP 2006316054 | A | 20061124 | JP 2006-111427 | 20060414 |
| PRIORITY APPLN. INFO.: | | | JP 2005-117662 | A 20050415 |
| OTHER SOURCE(S): | MARPAT | 145:505447 | | |

GI



AB Title openers, useful for prophylactic and therapeutic treatment of urinary frequency, incontinence, asthma, and chronic obstructive pulmonary disease, are prepared from tricyclic compds. I [ring A = benzene, heterocycle; ring B = benzene, heterocycle, cycloalkane, cycloalkene; ring

Updated Search

10540421

Q = halo- or (halo)alkyl-substituted pyrazole, isoxazole; R1, R3 = R5R6NCO, R5ONR6CO, R5R6NNHCO, R5CO, R5O, R5S, H, etc; R2, R4 = O, cyano, NO2, OH, alkoxy, halo, CO2H, etc.; R5, R6 = H, (un)substituted alkyl, (condensed) (un)substituted cycloalkyl, (un)substituted heterocyclyl, etc.; m, n = 0-2] are prepared Thus, deprotection of BOC-protected pyrazole derivative II (R = BOC) gave II (R = H), which inhibited K-induced bladder contraction with IC50 value of 1-3 μ M.

IT 850832-10-9P

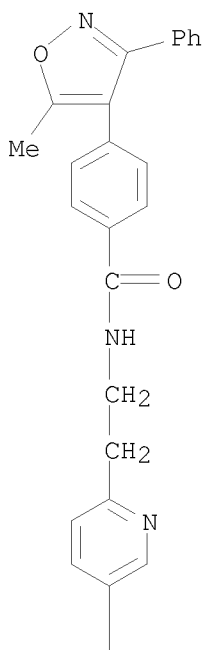
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrazoles or isoxazoles as high-conductance, Ca2+-sensitive K+ channel openers for treatment of diseases)

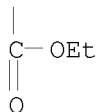
RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

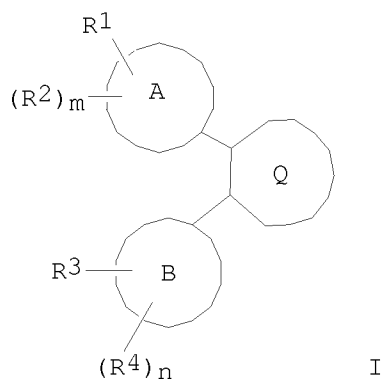


10540421

ACCESSION NUMBER: 2005:369275 HCAPLUS
DOCUMENT NUMBER: 142:430265
TITLE: Preparation of substituted pyrazoles and isoxazoles as
large conductance Ca-activated K channel openers
INVENTOR(S): Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki;
Hosaka, Toshihiro; Kono, Rikako
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 224 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|------------|
| ----- | --- | ----- | ----- | ----- |
| WO 2005037271 | A2 | 20050428 | WO 2004-JP15662 | 20041015 |
| WO 2005037271 | A3 | 20050901 | | |
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| RW: | BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
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| US 2007060629 | A1 | 20070315 | US 2006-574529 | 20060404 |
| PRIORITY APPLN. INFO.: | | | JP 2003-357325 | A 20031017 |
| | | | JP 2004-17662 | A 20040126 |
| | | | JP 2004-85143 | A 20040323 |
| | | | JP 2004-194172 | A 20040630 |
| | | | US 2004-584451P | P 20040701 |
| | | | WO 2004-JP15662 | W 20041015 |
| OTHER SOURCE(S): | CASREACT 142:430265; MARPAT 142:430265 | | | |
| GI | | | | |

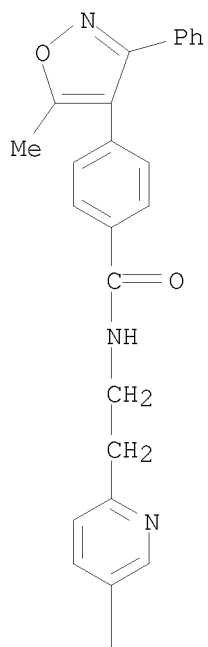
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- AB Title compds. I [A = benzene, heterocycle; B = benzene, heterocycle, etc.; Q = pyrazolyl, isoxazolyl; R1, R3 = carboxamido, hydrazido, etc.; m, n = 0-2; R2, R4 = oxo, CN, NO₂, etc.] are prepared For instance, 4,4,4-trifluoro-1-(4-methylphenyl)butane-1,3-dione is reacted with 3-methylphenylhydrazine•HCl (EtOH, reflux, 20 h) to give 1-(3-methylphenyl)-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazole (II). Data for over 400 compds. is given. The relaxation effect on K-induced contraction of isolated rabbit urinary bladder and the inhibitory effect on the rhythmic bladder contractions induced by substance P in anesthetized rats is provided for selected example compds. I are useful for the treatment of pollakiuria, urinary incontinence, etc.
- IT 850832-10-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of substituted pyrazoles and isoxazoles as large conductance Ca-activated K channel openers)
- RN 850832-10-9 HCAPLUS
- CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

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